

CHM 6470: *Chemical Bonding and Spectra*

Fall 2013 (3 credits)

Instructor: Nick Polfer, Chemistry Lab Building (CLB) 311C,
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Dr Polfer TBA

Office hours:

Lectures: T, R **2nd–3rd** period (8:30-10:25 am) TUR 2341

Aims: To provide students with a solid background in the concepts of quantum mechanics, to provide a deeper understanding of computational chemistry and relating these insights to spectroscopy.

Text book: *Molecular Quantum Mechanics*, by Atkins & Friedman (Oxford University Press)

Home work: Problem sets will be made available throughout the semester, which will be graded.

Exams: The course consists of one in-class exam during the semester as well as a comprehensive final. The exams will cover homework problems and will emphasize understanding of the lecture material and problem solving. All exams will be closed book.

Exam I Oct 8

Final comprehensive exam Dec 3

Grading:

The grade consists of four different types of assessments: exams (during-term and final), homework, attendance, and a project. The **during-term exam** is worth **20%**. The **final comprehensive exam** is also worth **20%**. The total points for the **homework** assignments are **35%** (5x7%). **Attendance** and active participation in class will be monitored for a score of 5%. A **project** is allocated a max of **20%**.

$$\text{Total} = 20 + 20 + 35 + 5 + 20 = 100\%$$

Proposed Grade Levels:

A:	92-100
A-:	88-91.9
B+:	84-87.9
B:	80-83.9
B-:	76-79.9
C+:	72-75.9
C:	68-71.9
C-:	64-67.9
D+:	60-63.9
D:	56-59.9
D-:	52-55.9
E:	< 52

Course policies:

Attendance in this course is expected. Any request for make-up exams should have a legitimate excuse, and be made to Dr. Polfer as far in advance as possible.

Students should also familiarize themselves with the UF Student Honor Code posted on the web at www.chem.ufl.edu/~itl/honor.html.

Students with disabilities must first register with the Dean of Students Office, see <http://www.chem.ufl.edu/~itl/disabilities.html>; the Dean of the Students Office will provide documentation to the student who must then provide this documentation to the instructor when requesting accommodation.

For counseling, students should consult the webpage: <http://www.chem.ufl.edu/~itl/counseling.html>

Advice:

We will cover **a lot of material** in a **short period of time**. It is hence essential that you keep up-to-date with the lecture material and do your homework assignments.

The lecture, homework exercises, example tutorial notebooks can be found on Sakai (<https://lss.at.ufl.edu/>) under the *Resources* tab. Lectures are named as follows, including the title: e.g. Lecture_1_Wave_Particle_Duality.pdf

Tentative Lecture Schedule CHM 6470

Lecture	Date	Topic	HW
	T 08/20	Chemistry Fall Departmental meeting	
1	R 08/22	Wave particle duality	
2	T 08/27	Dirac notation	
3	R 08/29	Commutators	
4	T 09/03	Uncertainty principle	
5	R 09/05	Schrödinger equation	
6	T 09/10	Particle in a 1 D box	H1
7	R 09/12	Harmonic oscillator	
8	T 09/17	Angular momentum	
9	R 09/19	The hydrogen atom	
10	T 09/24	Coupled 2-state system	
11	R 09/26	Spin and coupling of angular momenta	H2
	T 10/01	Review week	
	R 10/03	Review week	
	T 10/08	EXAM I	
12	R 10/10	Approximation methods: variational theorem	
13	T 10/15	Approximation methods: perturbation theory & time-dependent	
14	R 10/17	Molecules: Born-Oppenheimer approx.	H3
15	T 10/22	Molecular orbitals, energy diagrams	
16	R 10/24	Group theory	
17	T 10/29	Spectroscopy & rotations	
18	R 10/31	Vibrational spectroscopy	H4
19	T 11/05	Electronic spectroscopy	
20	R 11/07	Calculations in quantum chemistry	
21	T 11/12	MP2, DFT, CNDO	
22	R 11/14	MP2, DFT, CNDO	
23	T 11/19	Comparison of theory and expt	H5
	R 11/21	Presentation of projects	
	T 11/26	Presentation of projects	
	R 11/28	Presentation of projects	
	T 12/03	FINAL EXAM (in-class)	